Phenol, 3-methoxy-5-(2-phenylethyl)-17635-59-5 | DTXSID80170114

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 52.9

Global applicability domain: Inside

Local applicability domain index: 4.98e-01

Confidence level: 6.24e-01

Nearest Neighbors from the Training Set

Image not found

Isoamyl ether Measured: 170 Predicted: 137 Image not found

Menthol

Measured: 10.8 Predicted: 23.5

Image not found

(1R,2S,5R)-(-)-Menthol Measured: 10.8 Predicted: 23.5

Image not found

Disulfoton
Measured: 219
Predicted: 151

Image not found

Isoprocarb
Measured: 8.91
Predicted: 13.6

Image not found

N,N-Diethylaniline Measured: 102 Predicted: 12.8